

4-Phenyltoluene
644-08-6 | DTXSID4047177

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 240

Global applicability domain: Inside

Local applicability domain index: 5.81e-01

Confidence level: 6.78e-01

Nearest Neighbors from the Training Set

Image not found

Propane, 1,3-dibromo-2,2-bis(bromomethyl)-

Measured: 87.1

Predicted: 134

Image not found

2,4,4-Trimethyl-1-pentene

Measured: 603

Predicted: 347

Image not found

2,5-Dimethyl-2,4-hexadiene

Measured: 209

Predicted: 175

Image not found

Camphene

Measured: 955

Predicted: 598

Image not found

4-Vinylcyclohexene

Measured: 166

Predicted: 158